1,10-Phenanthroline 66-71-7 | DTXSID1025857

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 12.0 days

Global applicability domain: Outside

Local applicability domain index: 4.02e-01

Confidence level: 7.89e-01

Nearest Neighbors from the Training Set

Image not found

Tetralin

Measured: 120 Predicted: 12.2

Image not found

1,4-Dimethylnaphthalene

Measured: 511 Predicted: 13.7

Image not found

1-Methylnaphthalene

Measured: 164 Predicted: 12.0

Image not found

2,3-Dimethylnaphthalene

Measured: 511 Predicted: 13.8